L10 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:119949 CAPLUS Full-text

DN 140:267029

TI Miniaturization of Cell-Based β -Lactamase-Dependent FRET Assays to Ultra-High Throughput Formats to Identify Agonists of Human Liver X Receptors

AU Chin, Jayne; Adams, Alan D.; Bouffard, Aileen; Green, Ahren; Lacson, Raul G.; Smith, Todd; Fischer, Paul A.; Menke, John G.; Sparrow, Carl P.; Mitnaul, Lyndon J.

CS Department of Atherosclerosis and Endocrinology, Merck Research Laboratories, Rahway, NJ, USA

SO Assay and Drug Development Technologies (2003), 1(6), 777-787 CODEN: ADDTAR; ISSN: 1540-658X

PB Mary Ann Liebert, Inc.

DT Journal

LA English

AB Activation of liver X receptors (LXRs) induces reverse cholesterol transport and increases high-d. lipoprotein cholesterol in vivo. Here, we describe novel, functional, homogeneous cell-based fluorescence resonance energy transfer assays for identifying agonists of LXRs using β -lactamase as the reporter gene. Stable Chinese hamster ovary cell lines expressing LXR α -GAL4 or LXR β -GAL4 fusion proteins that regulate β -lactamase transcription from upstream 7 + UAS GAL4 DNA binding sequences were generated and characterized. Synthetic and natural ligands of LXR dose-dependently activated the expression of β -lactamase in a subtype-specific manner. These assays were used to demonstrate that a 1-pyridyl hydantoin small mol. LXR synthetic ligand specifically activates LXR α receptors. The β -lactamase assays were optimized for cell d., DMSO sensitivity, and time of agonist stimulation. Clonal LXR β -GAL4- β -lactamase cells were miniaturized into an ultra high throughput (3,456-well nanoplates) screening format.

IT 652992-38-6

RL: BSU (Biological study, unclassified); BUU (Biological use, unclassified); PRP (Properties); BIOL (Biological study); USES (Uses) (FRET assays were used to demonstrate that a 1-pyridyl hydantoin small mol. LXR synthetic ligand specifically activates LXR α receptors.)

RN 652992-38-6 CAPLUS

CN 2,4-Imidazolidinedione, 3-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]-1-(2-pyridinyl)- (9CI) (CA INDEX NAME)

RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

E gap ?

- AN 2004:101150 CAPLUS Full-text
- DN 140:146124
- TI Preparation of benzisoxazoles as LXR ligands for treating dyslipidemic conditions
- IN Jones, A. Brian; Adams, Alan D.; Green, Ahren I.; Huang, Shaei Y.; Tse, Bruno; Gutteridge, Clare E.; Cheng, Yuan
- PA Merck & Co., Inc., USA
- SO PCT Int. Appl., 134 pp.
- CODEN: PIXXD2
- DT Patent
- LA English
- FAN.CNT 1

FAN.				KIND DATE			APPLICATION NO.						DATE					
ΡI				A1 20040205		WO 2003-US22807						20030721						
		W:	ΑE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	ΒZ,	CA,	CH,	CN,
			CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,
			GM,	HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KR,	ΚZ,	LC,	LK,	LR,	LS,
			LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NI,	NO,	NZ,	OM,	PG,
			PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,	ТJ,	TM,	TN,	TR,
			TT,	TZ,	UA,	UG,	US,	UZ,	VC,	VN,	YU,	ZA,	ZM,	ZW				
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			BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG
	EP 1534696			A1 20050601			EP 2003-771693					20030721						
		R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,
			IE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	AL,	TR,	BG,	CZ,	EE,	HU,	SK	
	US 2005239769			A1 20051027			US 2005-522114						20050124					
PRAI	US	2002	-398	716P		P		2002	0725									
•	WO	2003	-US2	2807		W		2003	0721									
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AB The present invention relates to novel benzisoxazoles (shown as I; variables defined below; e.g. II) as LXR (nuclear oxysterol receptor) ligands and the pharmaceutically acceptable salts, esters and tautomers thereof, which are useful in the treatment of dyslipidemic conditions, particularly depressed

II

levels of HDL cholesterol. Although the methods of preparation are not claimed, .apprx.60 example prepns. of I and intermediates are included. example, II was prepared from pyrrolidine-2,5-dione and 7-propyl-3-neopentyl-6-(3-bromopropyloxy)-1,2-benzisoxazole in DMF in the presence of Cs2CO3 at room temperature; 7-propyl-3-neopentyl-6-(3- bromopropyloxy)-1,2-benzisoxazole was prepared from 6-hydroxy-7-propyl-3- neopentyl-1,2-benzisoxazole, 1,3dibromopropane and Cs2CO3 in DMF. The tested I have an IC50 ≤2 µM for at least one of either the LXR α or LXR β receptors employing the LXR radioligand competition scintillation proximity assays described. Examples of I tested for LXR transactivation have an EC50 of <5,500 nM for at least one of LXRa or LXRB receptor. Two examples of I were tested for their ability to increase cholesterol efflux from cultured human cells and the results are tabulated. For I: R1 = CF3, CH2CMe3, Ph, C1-6 alkyl, and C1-2-alkylphenyl; R2 = C1-6 alkyl, COOR3, CR3R4OR5, CR3R4SR5, and COR3; R3, R4 and R5 = H, Ph, and C1-6 alkyl; Y is joined together with the N and the carbonyl C shown in I to which Y is resp. attached, to form a heterocyclic ring = 5-membered rings (2oxopyrrolidin-1-yl, 2-oxoimidazolidin-1-yl, 4-oxoimidazolidin-1-yl, 2oxothiazolidin-3-yl, 4-oxothiazolidin-1-yl), 6-membered rings (2-oxopiperidin-1-yl, 3-oxomorpholin-4-yl, 2-oxohexahydropyrimidin-1-yl, 6-oxo-1,2,3,6tetrahydropyrimidin-1-yl, 2-oxohexahydropyrimidin-1-yl, 2-oxo-1,2,3,6tetrahydropyrimidin-1-yl, 2-oxopiperazin-1-yl, 2-oxohexahydrotriazin-1-yl, 2oxoazepan-1-yl), bicyclic heterocycles (phthalimido and related imides); Z = -C1-6alkyl-, -C1-6alkyl-O-, -C3-6cycloalkyl-, and -C3-6cycloalkyl-O-.

(drug candidate, chromatog. resolution; preparation of benzisoxazoles as

LXR

ligands for treating dyslipidemic conditions)

RN 652992-50-2 CAPLUS

CN 2,4-Imidazolidinedione, 5-methyl-3-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]-5-(2-pyridinyl)- (9CI) (CA INDEX NAME)

(drug candidate; preparation of benzisoxazoles as LXR ligands for treating dyslipidemic conditions)

RN 652992-51-3 CAPLUS

CN 2,4-Imidazolidinedione, 5-methyl-3-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]-5-(2-pyridinyl)-, (5S)-.(9CI) (CA INDEX NAME)

Absolute stereochemistry.

652992-59-1P, 1-[3-[[7-Propyl-3-(trifluoromethyl)-1,2-benzisoxazol6-yl]oxy]propyl]imidazolidin-2-one 652992-60-4P, Methyl
2-[2-oxo-3-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6yl]oxy]propyl]imidazolidin-1-yl]propanoate 652992-82-0P,
6-Phenyl-3-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6yl]oxy]propyl]dihydropyrimidine-2,4(1H,3H)-dione 652992-83-1P,
5-Methyl-3-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6yl]oxy]propyl]dihydropyrimidine-2,4(1H,3H)-dione
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP
(Preparation); RACT (Reactant or reagent); USES (Uses)
 (drug candidate; preparation of benzisoxazoles as LXR ligands for treating dyslipidemic conditions)

RN 652992-59-1 CAPLUS

CN 2-Imidazolidinone, 1-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]- (9CI) (CA INDEX NAME)

HN
$$N \longrightarrow (CH_2)_3 \longrightarrow 0$$
 $N \longrightarrow CF_3$

RN 652992-60-4 CAPLUS

CN 1-Imidazolidineacetic acid, α-methyl-2-oxo-3-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]-, methyl ester (9CI) (CA INDEX NAME)

MeO-C-CH N (CH2) 3-0
$$N$$
 CF3

RN 652992-82-0 CAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, dihydro-6-phenyl-3-[3-[[7-propyl-3-

(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]- (9CI) (CA INDEX NAME)

RN 652992-83-1 CAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, dihydro-5-methyl-3-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]- (9CI) (CA INDEX NAME)

IT 652992-23-9P, 1-[3-[[7-Propyl-3-(neopentyl)-1,2-benzisoxazol-6yl]oxy]propyl]pyrrolidine-2,5-dione 652992-24-0P, 1-[3-[[7-Propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6yl]oxy]propyl]pyrrolidine-2,5-dione 652992-25-1P, 2-[3-[[7-Propyl-3-(neopentyl)-1,2-benzisoxazol-6-yl]oxy]propyl]-1Hisoindole-1,3(2H)-dione 652992-26-2P, 3,3-Dimethyl-1-[3-[[7propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]pyrrolidine-2,5-dione 652992-27-3P, 3-Methyl-3-phenyl-1-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]pyrrolidine-2,5-dione 652992-28-4P, 3-[3-[[7-Propyl-3-(neopentyl)-1,2-benzisoxazol-6yl]oxy]propyl]thiazolidine-2,4-dione 652992-29-5P, 3-[3-[[7-Propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6yl]oxy]propyl]thiazolidine-2,4-dione 652992-30-8P, 5,5-Dimethyl-3-[3-[7-propyl-3-(neopentyl)-1,2-benzisoxazol-6yl]oxy]propyl]thiazolidine-2,4-dione 652992-31-9P, [2,4-Dioxo-3-[3-[7-propyl-3-(neopentyl)-1,2-benzisoxazol-6-yl]oxy]propyl]-1,3-thiazolidin-5-yl]acetic acid 652992-33-1P, 3-[3-[[7-Propyl-3-(neopentyl)-1,2-benzisoxazol-6yl]oxy]propyl]imidazolidine-2,4-dione 652992-34-2P, 3-[3-[[7-Propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6yl]oxy]propyl]imidazolidine-2,4-dione 652992-35-3P, 1-Methyl-3-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6yl]oxy]propyl]imidazolidine-2,4-dione 652992-36-4P, 5-(R)-Methyl-3-[3-[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6yl]oxy]propyl]imidazolidine-2,4-dione 652992-37-5P, 5,5-Dimethyl-3-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6yl]oxy]propyl]imidazolidine-2,4-dione 652992-38-6P, 1-(2-Pyridyl)-3-[3-[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6yl]oxy]propyl]imidazolidine-2,4-dione 652992-41-1P, 5-Methyl-5-phenyl-3-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-

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yl]oxy]propyl]imidazolidine-2,4-dione 652992-42-2P,
5-Methyl-5-phenyl-3-[3-[(7-propyl-3-(neopentyl)-1,2-benzisoxazol-6-
yl]oxy]propyl]imidazolidine-2,4-dione 652992-43-3P,
5-Methyl-5-phenyl-3-[3-[(7-propyl-3-phenyl-1,2-benzisoxazol-6-
yl]oxy]propyl]imidazolidine-2,4-dione 652992-44-4P,
5-Methyl-5-phenyl-3-[4-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-
yl]oxy]butyl]imidazolidine-2,4-dione 652992-45-5P,
5-Methyl-5-(3-carboxyphenyl)-3-[3-([7-propyl-3-(trifluoromethyl)-1,2-
benzisoxazol-6-yl]oxy]propyl]imidazolidine-2,4-dione 652992-48-8P
, 5-Methyl-5-(4-pyridyl)-3-[3-[[7-propyl-3-(trifluoromethyl)-1,2-
benzisoxazol-6-yl]oxy]propyl]imidazolidine-2,4-dione 652992-49-9P
, 5-Methyl-5-(3-pyridyl)-3-[3-[[7-propyl-3-(trifluoromethyl)-1,2-
benzisoxazol-6-yl]oxy]propyl]imidazolidine-2,4-dione 652992-52-4P
, 3-[3-[[7-Propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]-1-
(pyrimidin-2-yl)imidazolidine-2,4-dione 652992-53-5P,
3-[3-[(7-Propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl)oxy]propyl]-1-
(pyrazin-2-yl)imidazolidine-2,4-dione 652992-54-6P,
3-[2,5-Dioxo-4-phenyl-1-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-
6-yl]oxy]propyl]imidazolidin-4-yl]propanoic acid 652992-55-7P,
4-[5,5-Dimethyl-2,4-dioxo-3-[3-[[7-propyl-3-(trifluoromethyl)-1,2-
benzisoxazol-6-yl]oxy]propyl]imidazolidin-1-yl]butanoic acid
652992-58-0P, 5-[5,5-Dimethyl-2,4-dioxo-3-[3-[[7-propyl-3-
(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]imidazolidin-1-
yl]pentanoic acid 652992-61-5P, 2-[2-0xo-3-[3-[[7-propyl-3-
(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]imidazolidin-1-
yl]propanoic acid 652992-62-6P, 1-[3-[[7-Propyl-3-
(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]imidazolidine-2,4-dione
652992-65-9P, 5,5-Dimethyl-1-[3-[[7-propyl-3-(trifluoromethyl)-1,2-
benzisoxazol-6-yl]oxy]propyl]imidazolidine-2,4-dione 652992-70-6P
, 1-[[trans-2-[[7-Propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-
yl]oxy]cyclohexyl]methyl]dihydropyrimidine-2,6(1H,3H)-dione
652992-72-8P, 1-[[trans-2-[[7-Propyl-3-(trifluoromethyl)-1,2-
benzisoxazol-6-yl]oxy]cyclopentyl]methyl]dihydropyrimidine-2,6(1H,3H)-
dione 652992-78-4P, 1-[4-[7-Propyl-3-(trifluoromethyl)-1,2-
benzisoxazol-6-yl]butyl]dihydropyrimidine-2,6(1H,3H)-dione
652992-80-8P, 5-Phenyl-3-[3-[[7-propyl-3-(trifluoromethyl)-1,2-
benzisoxazol-6-yl]oxy]propyl]dihydropyrimidine-2,4(1H,3H)-dione
652992-85-3P, 1,5-Dimethyl-3-{3-[[7-propyl-3-(trifluoromethyl)-1,2-
benzisoxazol-6-ylloxylpropylldihydropyrimidine-2,4(1H,3H)-dione
652992-92-2P, 1-Phenyl-3-[3-[[7-propyl-3-(trifluoromethyl)-1,2-
benzisoxazol-6-yl]oxy]propyl]dihydropyrimidine-2,4(1H,3H)-dione
652992-96-6P, 3-[3-[[7-Propyl-3-(trifluoromethyl)-1,2-benzisoxazol-
6-yl]oxy]propyl]-1-pyridin-2-yldihydropyrimidine-2,4(1H,3H)-dione
652993-00-5P, 3-[3-[[7-Propyl-3-(trifluoromethyl)-1,2-benzisoxazol-
6-yl]oxy]propyl]-5,6-dihydro-2H-1,2'-bipyrimidine-2,4(3H)-dione
652993-04-9P, 3-[3-[[7-Propyl-3-(trifluoromethyl)-1,2-benzisoxazol-
6-yl]oxy]propyl]-5,6-dihydro-2H-1,5'-bipyrimidine-2,4(3H)-dione
652993-06-1P, 1-[3-[[7-Propyl-3-(neopentyl)-1,2-benzisoxazol-6-
yl]oxy]propyl]piperidin-2-one 652993-08-3P, 1-[3-[[7-Propyl-3-
(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]piperidin-2-one
652993-10-7P, 1-[3-[[7-Propyl-3-(trifluoromethyl)-1,2-benzisoxazol-
6-yl]oxy]propyl]piperidin-2,6-dione 652993-13-0P,
1-[3-[[7-Propyl-3-phenyl-1,2-benzisoxazol-6-yl]oxy]propyl]piperidin-2,6-
dione 652993-15-2P, 4-[3-[[7-Propyl-3-(trifluoromethyl)-1,2-
benzisoxazol-6-yl]oxy]propyl]morpholine-3,5-dione 652993-17-4P,
1-[3-[[7-Propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-
yl]oxy]propyl]piperazine-2,5-dione 652993-20-9P,
3-[3-[[7-Propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]-
1,3,5-triazinane-2,4-dione 652993-22-1P, 3-[3-[[7-Propyl-3-
phenyl-1,2-benzisoxazol-6-yl]oxy]propyl]dihydropyrimidine-2,4(1H,3H)-dione
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652993-23-2P, 6-Methyl-3-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]dihydropyrimidine-2,4(1H,3H)-dione 652993-24-3P, 1-[3-[[7-Propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]azepan-2-one 652993-25-4P, 1-Phenyl-3-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]imidazolidine-2,4-dione RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(drug candidate; preparation of benzisoxazoles as LXR ligands for treating dyslipidemic conditions)

RN 652992-23-9 CAPLUS

CN 2,5-Pyrrolidinedione, 1-[3-[[3-(2,2-dimethylpropyl)-7-propyl-1,2-benzisoxazol-6-yl]oxy]propyl]- (9CI) (CA INDEX NAME)

RN 652992-24-0 CAPLUS

CN 2,5-Pyrrolidinedione, 1-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]- (9CI) (CA INDEX NAME)

RN 652992-25-1 CAPLUS

CN 1H-Isoindole-1,3(2H)-dione, 2-[3-[[3-(2,2-dimethylpropyl)-7-propyl-1,2-benzisoxazol-6-yl]oxy]propyl]- (9CI) (CA INDEX NAME)

RN 652992-26-2 CAPLUS

CN 2,5-Pyrrolidinedione, 3,3-dimethyl-1-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]- (9CI) (CA INDEX NAME)

RN 652992-27-3 CAPLUS

CN 2,5-Pyrrolidinedione, 3-methyl-3-phenyl-1-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]- (9CI) (CA INDEX NAME)

RN 652992-28-4 CAPLUS

CN 2,4-Thiazolidinedione, 3-[3-[[3-(2,2-dimethylpropyl)-7-propyl-1,2-benzisoxazol-6-yl]oxy]propyl]- (9CI) (CA INDEX NAME)

RN 652992-29-5 CAPLUS

CN 2,4-Thiazolidinedione, 3-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]- (9CI) (CA INDEX NAME)

RN 652992-30-8 CAPLUS

CN 2,4-Thiazolidinedione, 3-[3-[[3-(2,2-dimethylpropyl)-7-propyl-1,2-benzisoxazol-6-yl]oxy]propyl]-5,5-dimethyl- (9CI) (CA INDEX NAME)

RN 652992-31-9 CAPLUS

CN 5-Thiazolidineacetic acid, 3-[3-[[3-(2,2-dimethylpropyl)-7-propyl-1,2-benzisoxazol-6-yl]oxy]propyl]-2,4-dioxo-(9CI) (CA INDEX NAME)

RN 652992-33-1 CAPLUS

CN 2,4-Imidazolidinedione, 3-[3-[[3-(2,2-dimethylpropyl)-7-propyl-1,2-benzisoxazol-6-yl]oxy]propyl]- (9CI) (CA INDEX NAME)

RN 652992-34-2 CAPLUS

CN 2,4-Imidazolidinedione, 3-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]- (9CI) (CA INDEX NAME)

RN 652992-35-3 CAPLUS

CN 2,4-Imidazolidinedione, 1-methyl-3-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]- (9CI) (CA INDEX NAME)

RN 652992-36-4 CAPLUS

CN 2,4-Imidazolidinedione, 5-methyl-3-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]-, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Me
$$C$$
 CH_2 CH_2 CH_3 CF_3

RN 652992-37-5 CAPLUS

CN 2,4-Imidazolidinedione, 5,5-dimethyl-3-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]- (9CI) (CA INDEX NAME)

RN 652992-38-6 CAPLUS

CN 2,4-Imidazolidinedione, 3-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]-1-(2-pyridinyl)- (9CI) (CA INDEX NAME)

RN 652992-41-1 CAPLUS

CN ' 2,4-Imidazolidinedione, 5-methyl-5-phenyl-3-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]- (9CI) (CA INDEX NAME)

RN 652992-42-2 CAPLUS

CN 2,4-Imidazolidinedione, 3-[3-[[3-(2,2-dimethylpropyl)-7-propyl-1,2-benzisoxazol-6-yl]oxy]propyl]-5-methyl-5-phenyl- (9CI) (CA INDEX NAME)

RN 652992-43-3 CAPLUS

CN 2,4-Imidazolidinedione, 5-methyl-5-phenyl-3-[3-[(3-phenyl-7-propyl-1,2-benzisoxazol-6-yl)oxy]propyl]- (9CI) (CA INDEX NAME)

RN 652992-44-4 CAPLUS

CN 2,4-Imidazolidinedione, 5-methyl-5-phenyl-3-[4-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]butyl]- (9CI) (CA INDEX NAME)

RN 652992-45-5 CAPLUS

CN Benzoic acid, 3-[4-methyl-2,5-dioxo-1-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]-4-imidazolidinyl]- (9CI) (CA INDEX NAME)

RN 652992-48-8 CAPLUS

CN 2,4-Imidazolidinedione, 5-methyl-3-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]-5-(4-pyridinyl)- (9CI) (CA INDEX NAME)

RN 652992-49-9 CAPLUS

CN 2,4-Imidazolidinedione, 5-methyl-3-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]-5-(3-pyridinyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c}
 & \text{N} & \text{CH2} \\
 & \text{N} & \text{CF3}
\end{array}$$

RN 652992-52-4 CAPLUS

CN 2,4-Imidazolidinedione, 3-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]-1-(2-pyrimidinyl)- (9CI) (CA INDEX NAME)

RN 652992-53-5 CAPLUS

CN 2,4-Imidazolidinedione, 3-[3-[[7-propyl-3-(trifluoromethyl)-1,2-

benzisoxazol-6-yl]oxy]propyl]-1-pyrazinyl- (9CI) (CA INDEX NAME)

RN 652992-54-6 CAPLUS

CN 4-Imidazolidinepropanoic acid, 2,5-dioxo-4-phenyl-1-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]- (9CI) (CA INDEX NAME)

RN 652992-55-7 CAPLUS

CN 1-Imidazolidinebutanoic acid, 5,5-dimethyl-2,4-dioxo-3-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]- (9CI) (CA INDEX NAME)

RN 652992-58-0 CAPLUS

CN 1-Imidazolidinepentanoic acid, 5,5-dimethyl-2,4-dioxo-3-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]- (9CI) (CA INDEX NAME)

CN l-Imidazolidineacetic acid, α -methyl-2-oxo-3-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]- (9CI) (CA INDEX NAME)

RN 652992-62-6 CAPLUS

CN 2,4-Imidazolidinedione, 1-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]- (9CI) (CA INDEX NAME)

RN 652992-65-9 CAPLUS

CN 2,4-Imidazolidinedione, 5,5-dimethyl-1-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]- (9CI) (CA INDEX NAME)

RN 652992-70-6 CAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, dihydro-3-[[(1R,2S)-2-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]cyclohexyl]methyl]-, rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 652992-72-8 CAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, dihydro-3-[[(1R,2S)-2-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]cyclopentyl]methyl]-, rel-(9CI) (CA INDEX NAME)

Relative stereochemistry.

RN 652992-78-4 CAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, dihydro-3-[4-[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]butyl]- (9CI) (CA INDEX NAME)

RN 652992-80-8 CAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, dihydro-5-phenyl-3-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]- (9CI) (CA INDEX NAME)

RN 652992-85-3 CAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, dihydro-1,5-dimethyl-3-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]- (9CI) (CA INDEX NAME)

RN 652992-92-2 CAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, dihydro-1-phenyl-3-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]- (9CI) (CA INDEX NAME)

RN 652992-96-6 CAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, dihydro-3-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]-1-(2-pyridinyl)- (9CI) (CA INDEX NAME)

RN 652993-00-5 CAPLUS

CN [1(2H),2'-Bipyrimidine]-2,4(3H)-dione, 5,6-dihydro-3-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]- (9CI) (CA INDEX NAME)

RN 652993-04-9 CAPLUS

CN [1(2H),5'-Bipyrimidine]-2,4(3H)-dione, 5,6-dihydro-3-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]- (9CI) (CA INDEX NAME)

RN 652993-06-1 CAPLUS

CN 2-Piperidinone, 1-[3-[[3-(2,2-dimethylpropyl)-7-propyl-1,2-benzisoxazol-6-yl]oxy]propyl]- (9CI) (CA INDEX NAME)

RN 652993-08-3 CAPLUS

CN 2-Piperidinone, 1-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]- (9CI) (CA INDEX NAME)

RN 652993-10-7 CAPLUS

CN 2,6-Piperidinedione, 1-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]- (9CI) (CA INDEX NAME)

RN 652993-13-0 CAPLUS

CN 2,6-Piperidinedione, 1-[3-[(3-phenyl-7-propyl-1,2-benzisoxazol-6-yl)oxy]propyl]- (9CI) (CA INDEX NAME)

RN 652993-15-2 CAPLUS

CN 3,5-Morpholinedione, 4-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]- (9CI) (CA INDEX NAME)

RN 652993-17-4 CAPLUS

CN 2,5-Piperazinedione, 1-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]- (9CI) (CA INDEX NAME)

RN 652993-20-9 CAPLUS

CN 1,3,5-Triazine-2,4(1H,3H)-dione, dihydro-3-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]- (9CI) (CA INDEX NAME)

RN 652993-22-1 CAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, dihydro-3-[3-[(3-phenyl-7-propyl-1,2-benzisoxazol-6-yl)oxy]propyl]- (9CI) (CA INDEX NAME)

RN 652993-23-2 CAPLUS

CN 2,4(1H,3H)-Pyrimidinedione, dihydro-6-methyl-3-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]- (9CI) (CA INDEX NAME)

RN 652993-24-3 CAPLUS

CN 2H-Azepin-2-one, hexahydro-1-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]- (9CI) (CA INDEX NAME)

RN 652993-25-4 CAPLUS

CN 2,4-Imidazolidinedione, 1-phenyl-3-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]- (9CI) (CA INDEX NAME)

 (Reactant or reagent)

(preparation of benzisoxazoles as LXR ligands for treating dyslipidemic conditions)

RN 652992-57-9 CAPLUS

CN 1-Imidazolidinebutanoic acid, 5,5-dimethyl-2,4-dioxo-3-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]-, ethyl ester (9CI) (CA INDEX NAME)

Eto-C-(CH₂) 3 N (CH₂) 3-0 N
$$\sim$$
 CF3

RN 652992-64-8 CAPLUS

CN 2,4-Imidazolidinedione, 3-[(4-methoxyphenyl)methyl]-1-[3-[[7-propyl-3-(trifluoromethyl)-1,2-benzisoxazol-6-yl]oxy]propyl]- (9CI) (CA INDEX NAME)

MeO
$$CH_2$$
 N $(CH_2)_{3-0}$ N CF_3

RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2000:314695 CAPLUS Full-text

DN 132:334473

TI Preparation of (carbamoylmethyl)pyrazinones as thrombin inhibitors

IN Sanderson, Philip E.; Lyle, Terry A.; Dorsey, Bruce D.; Stanton, Matthew G.; Staas, Donnette; Coburn, Craig; Naylor-Olsen, Adel M.; Morrissette, Matthew M.; Selnick, Harold G.; Nanterment, Philippe G.; Williams, Peter D.; Stauffer, Kenneth J.; Burgey, Christopher; Isaacs, Richard

PA Merck & Co., Inc., USA; Barrow, James, C.

SO PCT Int. Appl., 210 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

1741.	PATENT NO.				KIND DATE				APPLICATION NO.									
ΡI	WO 2000026211							WO 1999-US25203										
		W:	ΑE,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	CA,	CH,	CN,	CR,	CU,
									FI,									
			IN.	IS,	JP.	KE,	KG,	KR,	KZ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	MA,	MD,
			•	•		•	•	•	NZ,	•	•	-	•	•	•	-		
			•	•	•	•	•	•	UA,	•	-	•	•	-	-	-		
			•	•	•	-	-	ТJ,	-	•		•	•	•	•	·	•	
		RW:	•	•	•	•	•	•	SL,	SZ.	TZ,	UG,	ZW,	AT,	BE,	CH,	CY,	DE,
			-						IE,									
			•	•	•	•			ML,	•	•				•	•	•	•
	CA	2348							0511							1	9991	028
	ΕP	1124	822															
									FR,									
			•	•	-	LV,		•	•	•	•	•	•		· · ·	•	•	•
	AU	7477	-	•	•	B2			0523		AU 2	000-	1599	7		1	9991	028
	JР	P 2002528543 T2 20020903				JP 2000-579599						19991028						
	US	6610	692			В1				US 1999-429741					19991028			
PRAI	US	1998	-106				19981030											
				5203 W 19991028					•									
OS MARPAT 132:334473																		
GT																		

The (carbamoylmethyl)pyrazinones I [wherein b = NY1 or O; c = CY2 or N; d = CY3 or N; e-g = CY4 or N; Y1 and Y2 = independently H, (cyclo)alkyl, halogen, NH2, OH, or alkoxy; Y3 = H, (cyclo)alkyl, halogen, CN, NH2, or alkoxy; Y4 = independently H, alkyl, or halogen; W = H, R1, R102C, R1CO, R1S02, R1(CH2)nNHCO, or (R1)2CH(CH2)nNHCO; n = 0-4; R1 = H, (un)substituted (cycloalkyl)alkyl, alkoxyalkyl, difluoroalkyl, carboxyalkyl, Ph, naphthyl, heterocyclyl, etc.; X = H or halogen; R3 = H, (cyclo)alkyl, halogen, (un)substituted Ph, acyl, heterocyclyl, CN, SMe, SOMe, or alkylsulfonyl] and its analogs were prepared I inhibited human α-thrombin and are expected to be useful as blood platelet aggregation inhibitors, thrombus formation

inhibitors, anticoagulants, and thrombolytics. Thus, 3-(2-phenylethylamino)-6-methyl-1- carboxymethylpyrazinone was amidated by 5-aminomethylindole in DMF in the presence of HOBT, EDC, and TEA to yield the

. (indolylmethylcarbamoylmethyl) pyrazinone II, which showed thrombin inhibitory activity with a Ki of \leq 20 nM.

IT 267874-82-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(target compound; preparation of

(heterocyclylmethylcarbamoylmethyl)pyrazinone

s as thrombin inhibitors)

RN 267874-82-8 CAPLUS

CN 1(2H)-Pyrazineacetamide, 6-methyl-N-[(3-methyl-1,2-benzisoxazol-5-yl)methyl]-2-oxo-3-[[2-(2-pyridinyl)ethyl]amino]- (9CI) (CA INDEX NAME)

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1989:614472 CAPLUS Full-text

DN 111:214472

TI Preparation of 3-piperidinyl-1,2-benzisoxazoles as psychotic drugs

IN Antoku, Fujio; Yoshigi, Mayumi; Saji, Ikutaro; Ishizumi, Kikuo

PA Sumitomo Pharmaceuticals Co., Ltd., Japan

SO Eur. Pat. Appl., 43 pp.

CODEN: EPXXDW

DT Patent

LA English

FAN.CNT 1

FAN.	CNT 1				
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	EP 314098	A2	19890503	EP 1988-117836	19881026
	EP 314098	A3	19900103		
	EP 314098	B1	19930804		
	R: AT, BE, CH,	DE, ES	, FR, GB, GR	, IT, LI, LU, NL, SE	
	JP 01199967	A2	19890811	JP 1988-266754	19881021
	CA 1335289	A1	19950418	CA 1988-581028	19881024
	US 4937249	· A	19900626	US 1988-262575	19881025
	AT 92489	E	19930815	AT 1988-117836	19881026
	ES 2059468	Т3	19941116	ES 1988-117836	19881026
PRAI	JP 1987-271462	Α	19871026		
	EP 1988-117836	Α	19881026	•	
os	MARPAT 111:214472				
GT		•			

$$Q^{2} = R^{1} \qquad \qquad R^{5} \qquad R^{3}$$

$$R^{2} \qquad \qquad R^{6} \qquad R^{3}$$

$$Q^{4} = R^{9}$$
 $Q^{5} = R^{11} - 1$ $(CH_2)_{n}$

The title compds. (I; A = CO, SO2; when A = CO, B = Q1-Q5; when A = SO2, B =AB 1,2-phenylene; R1 = R2 = H; or either one of R1, R2 = H, the other = OH, C1-5 alkyl, C2-6 alkanoyloxy; R1R2 $\stackrel{\cdot}{=}$ O; E = O, CH2, CH2CH2; F = CH2, CH2CH2; R3-R8 = H, C1-5 alkyl; R9-R12 = C1-5 alkyl; R11R12 = C3-5 alkylene; n = 0-2; W = C1-6 alkylene, C2-6 alkenylene, C2-6 alkynylene, C2-6 hydroxyalkylene; G = H, C1-5 alkyl, C1-5 alkoxy, halo, HO) were prepared as psychotic drugs useful as highly selective neuroleptics, active also as analgesics, allergy inhibitors, and cardiovascular agents. A mixture of N-(4bromobutyl)cyclohexane-1,2-dicarboximide, 3-(4-piperidinyl)-6- fluoro-1,2benzisoxazole, K2CO3, and KI in DMF was heated 11 h at 90-100° to give 72.8% N-[4-[4-(6-fluoro-1,2-benzisoxazol-3-yl)piperidinyl]butyl]cyclohexane-1,2dicarboximide (II). In a test for neuroleptic activity against pos. symptoms, II suppressed the climbing behavior in mice induced by apomorphine with an ED50 of 0.92 mg/kg after 1 h, vs. 1.8 and 9.4 mg/kg for chlorpromazine and tiaspirone, resp.

IT 123547-84-2P 123547-85-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological

study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of, as antipsychotic)

RN 123547-84-2 CAPLUS

CN

1H-Isoindole-1,3(2H)-dione, hexahydro-2-[4-[4-(6-methyl-1,2-benzisoxazol-3-yl)-1-piperidinyl]butyl]-, monohydrochloride (9CI) (CA INDEX NAME)

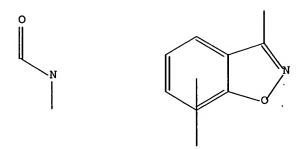
RN 123547-85-3 CAPLUS

CN 4,7-Methano-1H-isoindole-1,3(2H)-dione, hexahydro-2-[4-[4-(6-methyl-1,2-benzisoxazol-3-yl)-1-piperidinyl]butyl]-, monohydrochloride, $(3a\alpha,4\beta,7\beta,7a\alpha)$ - (9CI) (CA INDEX NAME)

Relative stereochemistry.

● HCl

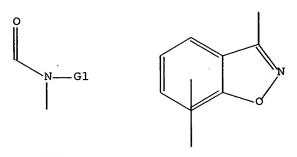
=> d 12; d 17; d his; log y L2 HAS NO ANSWERS L1 STR



Structure attributes must be viewed using STN Express query preparation. L2 QUE ABB=ON PLU=ON L1

L7 HAS NO ANSWERS

L6 STR



G1 Cb,Ak

Structure attributes must be viewed using STN Express query preparation. L7 QUE ABB=ON PLU=ON L6

(FILE 'HOME' ENTERED AT 09:59:44 ON 10 NOV 2005)

FILE 'REGISTRY' ENTERED AT 09:59:53 ON 10 NOV 2005

L1 STRUCTURE UPLOADED

L2 QUE L1

L3 2 S L2

L4 . 76 S L2 FUL

FILE 'CAPLUS' ENTERED AT 10:00:16 ON 10 NOV 2005

L5 , 12 S L4

FILE 'REGISTRY' ENTERED AT 10:00:23 ON 10 NOV 2005

L6 STRUCTURE UPLOADED

L7 QUE L6

L8 2 S L7 SAM SUB=L4

L9 63 S L7 FUL SUB=L4

FILE 'CAPLUS' ENTERED AT 10:01:37 ON 10 NOV 2005

L10 4 S L9

COST IN U.S. DOLLARS SINCE FILE TOTAL
ENTRY SESSION
FULL ESTIMATED COST 20.21 221.11

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION

CA SUBSCRIBER PRICE -2.92 -2.92

STN INTERNATIONAL LOGOFF AT 10:02:26 ON 10 NOV 2005